



From Quantum Mechanics to Force Fields

By Jean-Philip Piquemal

Springer-Verlag GmbH Feb 2013, 2013. Buch. Condition: Neu. Neuware - The authors of this volume illustrate recent trends in the design and application of accurate force fields. 15 papers reflect the present questions including the strategies for (i) the inclusion of the polarization energy and (ii) an optimal parametrization of models. They highlight the directions to follow as new exciting fields of application emerge. Expert authors discuss the optimization and parametrization of new models, put in perspectives the actual importance of the polarization energy, as well as review or propose new models explicitly for incorporating polarization. They also present models that are applied to difficult systems or challenging fields of application. Originally published in the journal Theoretical Chemistry Accounts, these outstanding contributions are now available in a hardcover print format. This volume is of benefit in particular to those research groups and libraries that have chosen to have only electronic access to the journal. It also provides valuable content for all researchers in theoretical chemistry. 204 pp. Englisch.



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